ECE 371
Materials and Devices

09/12/19 - Lecture 7

Formation of Energy Bands and
Kronig-Penney Model

General Information

- Homework #2 due today before class
- Homework #3 assigned, due Tuesday 10/1
- First midterm (covers Ch. 1 and Ch. 2) is on Tuesday 9/24
- Midterm will be closed book/notes and consist of:
  - 5-10 multiple choice questions on Ch. 1 and Ch. 2 material
  - 1 question on crystal planes/lattices
  - 2 questions on quantum mechanics
  - Some relevant equations and constants will be provided
  - Calculators okay
- I will hold a midterm review session and record it. Time and location TBD. Look for an email.
- Previous midterm questions will be posted on the course website on UNM Learn.
- Reading for next time: 3.1

Energy Level Splitting for Electrons

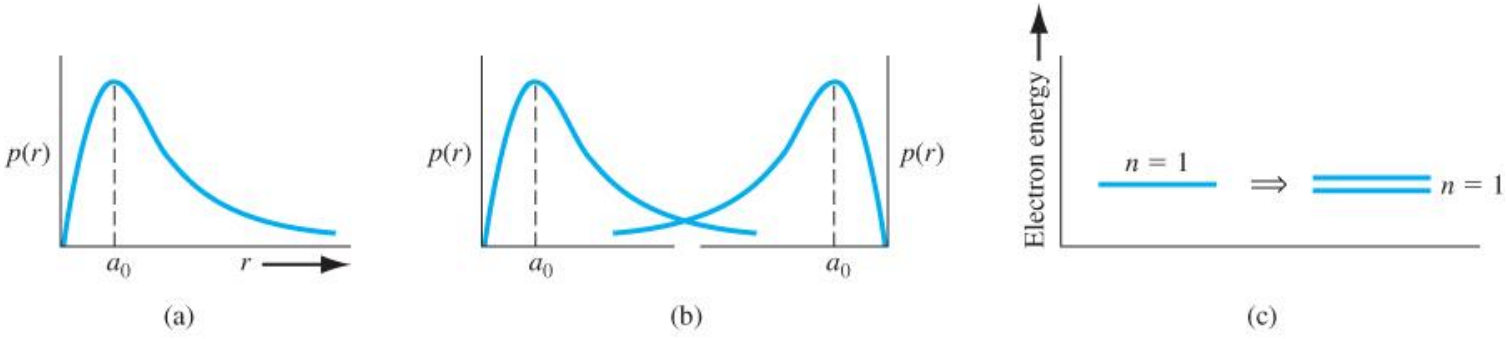

Figure 3.1 | (a) Probability density function of an isolated hydrogen atom. (b) Overlapping probability density functions of two adjacent hydrogen atoms. (c) The splitting of the $n = 1$ state.

- In atoms, electron energy levels are quantized
- Electron location has associated probability density function
- When two electrons are spatially close, their wave functions overlap and a perturbation (small change) in their energy levels occurs
- Solution to the Schrodinger equation for two interacting electrons leads to a splitting in their energies ($E \rightarrow E_0 - A \; and \; E_0 + A$)
- Splitting consistent with Pauli exclusion principle but *not caused* by it

Formation of Energy Bands

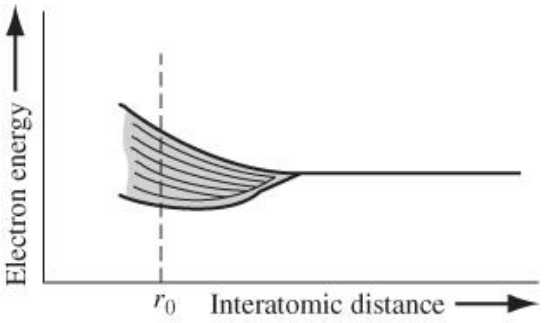

Figure 3.2 | The splitting of an energy state into a band of allowed energies.

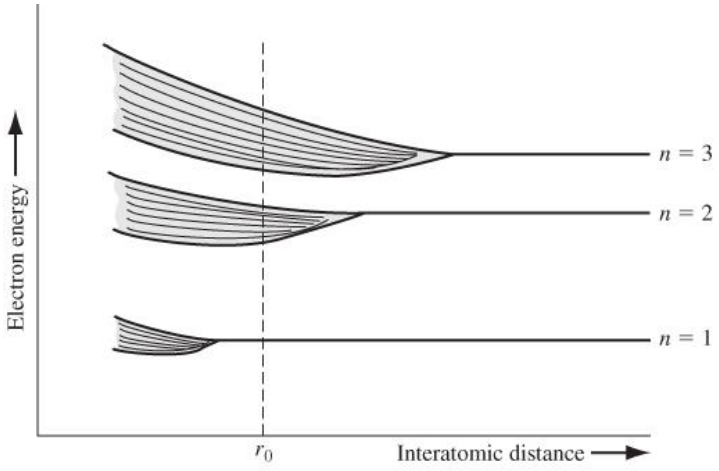

Figure 3.3 | Schematic showing the splitting of three energy states into allowed bands of energies.

- Separated atoms ⇒ No interactions ⇒ no splitting
- When atoms move closer together to their equilibrium lattice spacing, the energy levels split
- For N-electrons, there is an N-fold splitting
- For real crystals (huge number of electrons!), a quasi continuous band of energies forms when the atoms (electrons) interact

Formation of Energy Bands

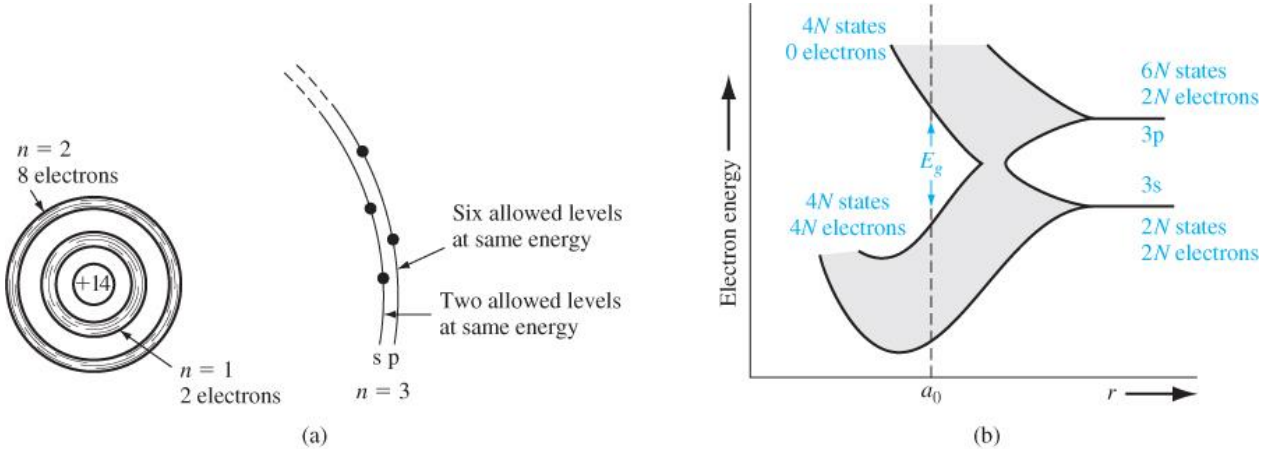

Figure 3.4 | (a) Schematic of an isolated silicon atom. (b) The splitting of the 3s and 3p states of silicon into the allowed and forbidden energy bands.
(From Shockley [6].)

- In silicon, only the electrons in the n = 3 valence shell interact
- Outer shell has s and p subshells with 2 and 2 atoms, respectively
- 2 interacting atoms ⇒ 8 interacting electrons ⇒ 4 original (degenerate) energy levels split into 8 levels (4 in the valence band, 4 in the conduction band)
- At 0K, all 8 electrons reside in the valence band ⇒ no conduction at 0K

Periodic Potentials

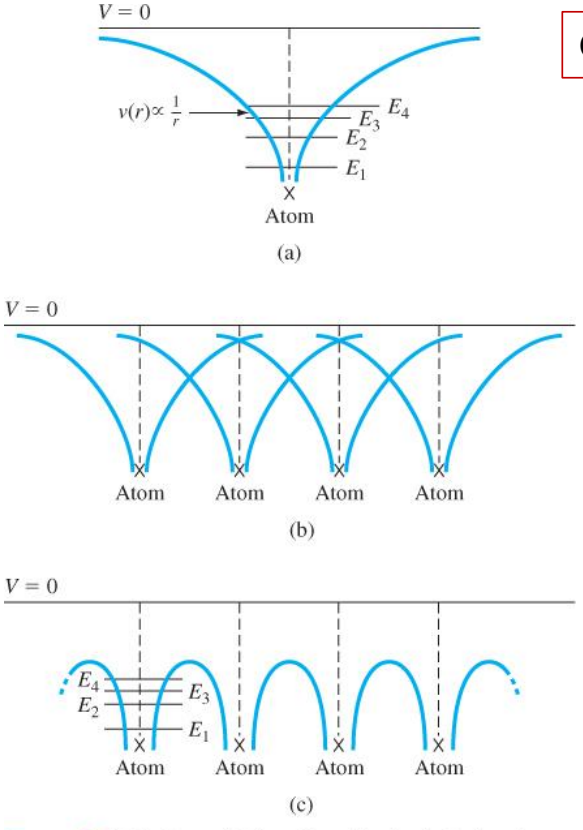

Figure 3.5 | (a) Potential function of a single isolated atom. (b) Overlapping potential functions of adjacent atoms. (c) Net potential function of a one-dimensional single crystal.

Goal: solve Schrodinger equation for a periodic potential

$$V(r) = \frac{1}{4\pi\varepsilon_0}\frac{q_1 q_2}{r}$$

*q is negative for an electron

- When electron and nucleus are far apart, the potential energy is zero
- As they move closer together, it becomes negative (implying we would need to add energy to the system to separate them)
- When atoms interact, the overall potential is lowered
- Real potential shape is difficult to solve analytically

Kronig-Penney Model

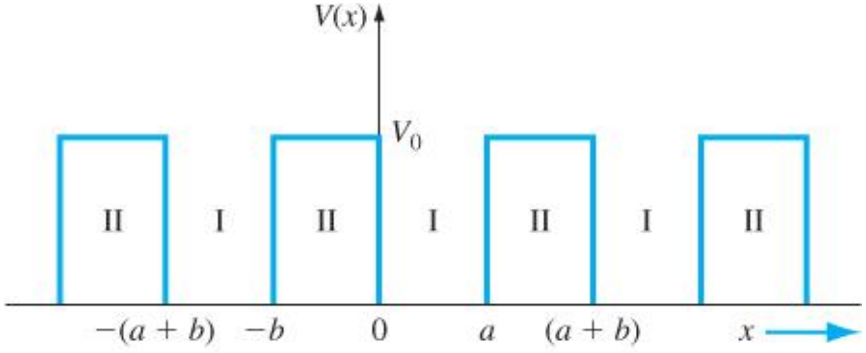

Figure 3.6 | The one-dimensional periodic potential function of the Kronig–Penney model.

- Use 1D array of periodic finite potential wells to model the potential in a crystal
- Solution to Schrodinger equation yields
  - Allowed energy bands
  - Forbidden energy gaps
  - E vs. k relationship (dispersion curve) for electrons
  - Effective mass (m*)
  - Holes (electrons behaving as positive charges)
- Examine the case when $E < V_0$ (electron bound by crystal)

*see in-class derivation

Bloch's Theorem

- Assumption that wave function will not deviate significantly from those of free electrons
- For a periodic potential Bloch showed the wave functions are of the form

$$\psi(x) = u(x)e^{jkx}$$

$u(x)$ is function that is periodic with the crystal lattice and modifies the amplitude

$$u(x) = u\big(x + (a+b)\big) = u\big(x + 2(a+b)\big) = \ \ldots$$

e^{jkx} is the wave function of a free electron

k is the constant of motion or wave number